ARMA 16-270

Breakage Mechanics Modeling of the Brittle-ductile Transition in Granular Materials

Wang, P., and Arson, C.

School of Civil and Environmental Engineering

Georgia Institute of Technology, Atlanta, Georgia, USA

ABSTRACT: During comminution, several energy dissipation processes operate simultaneously, including plastic work due to internal friction, fracture energy release due to particle breakage, and plastic work due to the rearrangement of fragments. Recent studies show that the plastic work due to particle rearrangement amounts to an important part in the total dissipated energy, which is much larger than the fracture energy released to create new surfaces, especially at high stress. This evolution of energy distribution between breakage dissipation and plastic work during the comminution of granular material manifests as a transition from brittleness to ductility. However, there is still no micromechanical model that can capture this transition. Breakage mechanics is a continuum mechanics theory that allows to analyzing the behavior of granular materials based on statistical and thermodynamic principles. We use this theory to propose a model that couples the energy dissipation caused by breakage and frictional plastic work. A friction plasticity parameter is coupled to the breakage parameter. Physically, the relationship between plasticity and breakage translates: (1) the increase of the dissipation induced by breakage in front of that induced by plastic deformation when fragments produced by breakage have rougher surfaces with higher friction angles than the non broken particles; and reversely; (2) the increase of the dissipation induced by plastic deformation in front of that induced by breakage when the multiplication of fragments results in higher particle coordination numbers, shielding effects and higher particle strength. Our modeling hypothesis is supported by experimental observations reported in the literature, and simulations show that our coupled breakage-plasticity model better captures the brittle-ductile transition observed in granular materials. The proposed modeling approach is expected to improve the fundamental understanding of quasi-static confined comminution, which is a major issue in civil engineering, powder technology and the mineral industry.

1. INTRODUCTION

The quasi-static confined comminution is used in civil engineering, powder technology and mineral industry. It is well known that during this process, particle movement and crushing will occur in order to increase the compressibility. Thus, the input energy will be dissipated by the plastic work due to friction and surface energy due to particle breakage [McDowell et al.,1996, Walsh and Tordesillas,2004]:

$$\delta W^p = \delta\Phi_p + \delta\Phi_B \tag{1}$$

where $\delta\Phi_p = Mp\delta\varepsilon$ and $\delta\Phi_B = \dfrac{\Gamma \mathrm{d}S}{V_s(1+e)}$ are obtained based on critical state soil mechanics. M is the slope of the critical state line; p is the effective mean stress; $\delta\varepsilon$ is the shear strain increment; Γ is the specific energy; V_s is volume of the material; and e is void ratio [McDowell, Bolton and Robertson,1996, Roscoe et al.,1963]. Recent studies further investigated the micro behavior during the comminution, and proposed that a dissipation due to the rearrangement of fragments ($\delta\Phi_{redist}$) accounts for a significant part in the total energy consumption. The ratio R of $\delta\Phi_{redist}$ and $\delta\Phi_B$ can be as large as 15 in the oedometric compression test [Russell,2011]. Another experiment by Ovalle suggests that the pure surface energy is predominant at low stresses and becomes less prominent at high stresses, when the redistribution of the particles produces large amount of plastic work [Ovalle et al.,2013]. It is also noted that $\delta\Phi_{redist}$ is also a kind of plastic work related to friction so that both $\delta\Phi_p$ and $\delta\Phi_{redist}$ can be seen as friction-plasticity dissipation potentials.

To better understand why a transition is observed from low to high pressures, let us consider a sample of granular material subject to an oedometer compression test. When the stress level is low, the stress is undertaken by the granular skeleton and thus leads to an increase in stored elastic energy. As the stress increases, friction occurs at some contacts. At this stage the coordination number of individual particles is low (compared to the coordination numbers noted in the crushed material). Therefore, when the stress in a particle reaches particle strength, mode I fracture propagation occurs and the granular assembly exhibits a brittle behavior [Wang et al.,2015, Tsoungui et al.,1999]. As the particles continue to break, both of the coordination number of the particles and the released surface energy increase. For high coordination numbers, particles become 'stronger' and exhibit ductile breakage. When the Particle Size Distribution (PSD) approaches the ultimate distribution [Coop et al.,2004], the probability of grain breakage decreases and energy dissipated by friction under high contact forces exceeds the surface energy released.

It can be concluded that breakage and plasticity dissipation processes are coupled, and what is called the redistribution energy is also a kind of plastic work that is the result of friction. Breakage dissipation dominates when the stress level is low while plastic dissipation dominates at higher stress.

In this paper, we formulate a breakage mechanics based model that couples the evolution of the PSD upon crushing with plastic parameters, in order to capture the transition from brittle to ductile behavior in granular media subjected to axial compression. The theory of breakage mechanics [Einav,2007] is based on the grain micromechanical behavior, PSD evolution laws and probability-based homogenization. In Section 2, we present the theoretical framework of our breakage-plasticity coupled model. In Section 3, we explain the computational algorithm that we used to predict the evolution of mechanical properties and microstructure upon crushing. In Section 4, simulations are presented to study the transition from brittleness to ductility during the compression of granular materials. A simple relationship is proposed to couple a frictional plastic parameter to the breakage variable.

2. THEORETICAL FORMULATION

Breakage mechanics is based on four fundamental assumptions [Das et al.,2011]:

- The elastic strain energy stored in the grains is linearly proportional to the grains' surface area;
- The ultimate particle size distribution (PSD) is fractal;
- Between the initial and the ultimate PSDs, the current PSD can be obtained by linear interpolation;
- The dissipation due to breakage is equal to the loss in residual breakage energy.

The balance of energy during the compression of a granular material can be expressed as [Einav,2007]:

$$\delta W = \delta\Psi + \delta\Phi \tag{2}$$

where δW is the work input provided at the boundaries ($\delta W = \sigma : \delta e$); Ψ (respectively $\delta\Psi$) is the Helmholtz free energy (respectively the increment of free energy); $\delta\Phi$ is the energy dissipated.

With the assumption that the energy stored in the grains is proportional to grains' surface area, the Helmholtz free energy is given by

$$\Psi = \psi_r(e_v^e)(1-\vartheta B) \tag{3}$$

where $\psi_r(e_v^e)$ the stored energy function; B is the breakage variable; and ϑ ranges from 0 to 1 and defines the distance from the initial to the ultimate grain size distribution.

In the elastic-plastic-breakage coupled model, the dissipation has the following expression:

$$\begin{aligned} \delta\Phi\left(B,\varepsilon_p\right) &= \delta\Phi_P\left(\varepsilon_p\right) + \delta\Phi_B\left(B\right) \\ \delta\Phi\left(B,\varepsilon_p\right) &= \sqrt{\delta\Phi_p^{*2}\left(B,\varepsilon_p\right) + \delta\Phi_B^{*2}\left(B,\varepsilon_p\right)}. \end{aligned} \tag{4}$$

$\delta\Phi_P$ and $\delta\Phi_B$ are the dissipation caused by the plasticity and breakage respectively. $\delta\Phi_p^{*2}$ and $\delta\Phi_B^{*2}$ are potentials that are defined to couple the two dissipation processes.

Then the balance equation Eq. (1) can be expressed as

$$\begin{aligned} &(\sigma - \psi_r(e_v^e)(1-\vartheta B)) : \delta e_e + (\sigma - \frac{\partial\delta\Phi}{\partial\delta e_p}) : \delta e_p \\ &+(\psi_r(e_v^e)\vartheta - \frac{\partial\delta\Phi}{\partial\delta B})\delta B = 0 \end{aligned} \tag{5}$$

A combined Legendre transformation provides:

$$y \equiv \sigma : \delta e_p + E_B\delta B - \delta\Phi \tag{6}$$

where E_B is the breakage energy ($\mathrm{E}_B = \psi_r(e_v^e)\vartheta$).

The following general yield surface is obtained

$$y \equiv \frac{\sigma:\sigma}{[\partial\delta\Phi_p^* / \partial\delta e_p]:[\partial\delta\Phi_p^* / \partial\delta e_p]} + \left(\frac{E_B}{\partial\delta\Phi_B^* / \partial B}\right)^2 - 1 \tag{7}$$

Eq.(7) implies that the plasticity yield surface and the breakage yield surface are coupled into a single surface. Then a simple model is proposed, such that:

$$\Phi_p^* = \sin^{-1}(\omega)\Phi_p; \Phi_B^* = \cos^{-1}(\omega)\Phi_B \quad (8)$$

where ω is the plastic-breakage coupling angle.

With Eq.(8), the yielding surface in Eq.(7) has the following form:

$$y = \left(\sin(\omega) \frac{\psi_r(e_v^e)\vartheta}{\xi(e_v^e)(1-\vartheta B)} p \right)^2 + (\cos(\omega)) - G_B(1-B)^{-4}. \quad (9)$$

In which:

$$p = \xi(e_v^e)(1-\vartheta B); \xi(e_v^e) = p_r\sqrt{K(1-m)(e_v^e - e_v^0)+1}, \quad (10)$$

Eq.(10) reduces to:

$$\begin{aligned} y &\equiv y_B = E_B - G_B(1-B)^{-2} \\ y &\equiv y_p = p - \frac{\xi(e_v^e)}{\psi_r(e_v^e)(1-B)^2\vartheta}. \end{aligned} \quad (11)$$

in which K, m and G_B are material constants.

3. COMPUTATIONAL METHOD

We built a computational algorithm based on the model described by Eq. (10). A confined test can be controlled in increments of strain or stress. At each loading step, δe_p and δB are then updated. In the algorithm proposed in the following, we assumed that the test was controlled in increments of volumetric strain (similar to an oedometric test). The strain increment at each loading step is given by:

$$\delta e_v = \delta e_v^e + \delta e_v^p \quad (12)$$

The consistency condition is expressed as:

$$Y(e_v, e_v^p, B) = \frac{\partial y}{\partial e_v}\delta e_v + \frac{\partial y}{\partial e_v^p}\delta e_v^p + \frac{\partial y}{\partial B}\delta B = 0 \quad (13)$$

where

$$\begin{aligned} &\frac{\partial y}{\partial e_v} \equiv \frac{\partial y_B}{\partial e_v} = \vartheta p_r \xi^{(1-m)}(e_v^e)(\mathrm{K}(1-\mathrm{m})(e_v^e - e_v^0)+1)^{\frac{m}{1-m}} \\ &\frac{\partial y}{\partial e_v} \equiv \frac{\partial y_p}{\partial e_p} = -\frac{\partial y}{\partial e_v} \\ &\delta e_v^p = \lambda\frac{\partial y}{\partial \sigma} = \frac{2\lambda \sin^2(\omega)}{p} \\ &\frac{\partial y}{\partial B} \equiv \frac{\partial y_B}{\partial B} = \frac{-2G_B}{(1-B)^3} \\ &\delta B = \lambda\frac{\partial y}{\partial E_B} = \frac{2\lambda\vartheta\cos^2(\omega)(1-\mathrm{B})^4\psi_r(e_v^e)}{G_B^2} \end{aligned} \quad (14)$$

At each loading step, the yield criterion is checked as follows:

$$\begin{cases} if\ y(e_v^{(k+1)}, e_v^{p(k)}, B^{(k)}) < 0 \\ \delta e_v^{p(k+1)} = 0;\ \delta B^{(k+1)} = 0 \\ if\ y(e_v^{(k+1)}, e_v^{p(k)}, B^{(k)}) > 0 \\ Y(e_v^{(k+1)}, e_v^{p(k)}, B^{(k)}) = 0 \Rightarrow \lambda, \delta e_v^{p(k+1)}, \delta B^{(k+1)} \end{cases} \quad (15)$$

Then, at each loading step, the terms of energy dissipation are calculated as follows:

$$\delta\Phi_p = p\delta e_v^{p(k+1)};\ \delta\Phi_B = G_B(1-B)^{-2}\delta B \quad (16)$$

After each step, the values of e_v, e_p, B, $\delta\Phi_p$ and $\delta\Phi_B$ are stored for the calculations to be performed in the following load steps.

4. SIMULATION

4.1. Parameters

The input parameters of the model presented in Section 3 include: the initial void ratio e_0, the maximum void ratio $\mathrm{e}_{\max}$, the material constants K, m and G_B, the coupling angle ω and the grading index ϑ. In the simulation presented in the following, we chose $\mathrm{e}_0 = 1.5$, $\mathrm{e}_{\max} = 1.8$, $\mathrm{K} = 3000$, $\mathrm{m} = 0.5$, $G_B = 10kPa$ and $\omega = 0^o,\ 40^o,\ 60^o,\ 80^o$ and 90^o.

4.2. Definition coupling angel ω as a function of breakage B

The coupling angle ω characterizes the distribution of dissipated energy between plastic work and breakage energy (surface energy) [Einav,2007]. ω is defined a linear function of the particle friction angle:

$$\omega = \alpha\phi \quad (17)$$

where α is a constant (which ranges from 1.6 to 3.4 for soils), and ϕ is the internal frictional angle of the dry granular material. In addition, ω is also expected to be related to the initial porosity of the granular assembly: higher porosity would result in a larger stress drop after a crushing event [Das, Nguyen and Einav,2011].

In our study, we assume that the angle ω changes with the breakage parameter B. To justify this hypothesis, let us consider a material with a small ω, therefore, a small friction angle. Particle breakage is the dominating dissipation process. For example, when a box of polished grass beads is subject to isotropic compression, dissipation occurs by particle crushing because glass beads are not angular and have a low friction coefficient. But as the glass beads begin to break, fragments will present rough surface, which will result in friction, and therefore, plastic dissipation due to friction. This means that the angle ω is not constant throughout the compression: it increases as the material becomes less brittle and more ductile. Another fact that justifies the dependence of the angle ω to the breakage parameter is the existence of an ultimate PSD $F_u(d)$: once the ultimate PSD is reached by successive crushing events, the breakage mechanics theory predicts that particles cannot break further because the increase of particle coordination number results in shielding effects, i.e. in a redistribution of compression contact forces into a quasi-hydrostatic stress distribution around particles[Wang and Arson,2016]. Consequently, as we approach $F_u(d)$ during the crushing process, it becomes harder to break particles, which means that the coupling angle ω should increase as breakage progresses.

As a starting point, we propose the following simple relationship between the plastic coupling angle and the breakage parameter:

$$\omega = \frac{\pi}{2} B. \tag{18}$$

This assumption is based on the idea that: (1) at the beginning of compression, particles have a low average coordination number, therefore breakage will not be impeded by shielding effects and friction dissipation will be limited due to the limited number of contacts and the relatively low confining stresses; (2) with the increased volumetric strain or stress, particles become 'stronger' due to larger coordination number (shielding effects) and are less likely to break, and the increased contact force generates more plastic work due to relative particle movement. Therefore, we model the brittle/ductile transition as a change of the angle ω from 0º ($B = 0$, brittle) to 90º ($B = 1$, ductile). In the following, we test our modeling hypothesis by comparing our coupled model (using Eq.(18)) to the model presented in Section 3, in which the coupling angle ω is a fixed parameter.

4.3. Simulation Results

Fig.1 shows the relationship between the volumetric stain and the effective mean stress p. The trend of the curve is typical of one-dimensional compression tests. With a fixed coupling angle ranging from 0º to 90º, the model varies from an elastic-breakage model to an elastic-perfect plastic model. It should be noted that with a fixed ω (except for ω=0º), a singular point exists at the transition from elastic to plastic/breakage, while for the proposed model with a varying ω, a continuous and differentiable curve is obtained.

Similar trends are obtained for the volumetric strain-breakage relationship, for both fixed and varying ω (Fig.2). The slopes of the curves decrease as breakage approaches to unity.

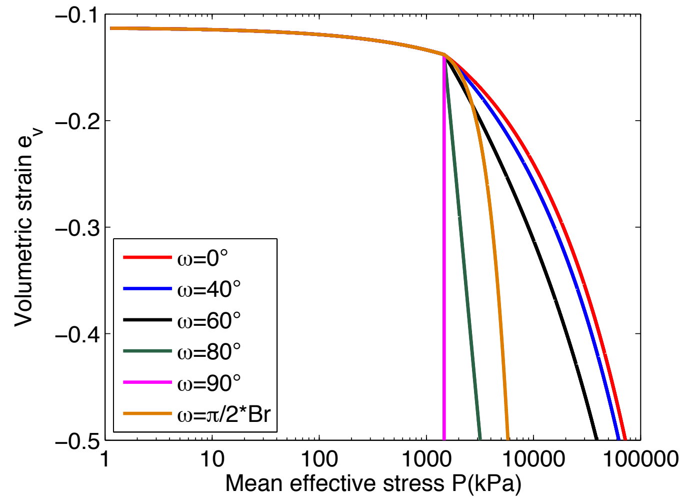

Fig. 1. The effect of the coupling angle ω on stress-strain relationship.

Fig.3 shows the ratio of plastic work and breakage dissipation. Before breakage happens, both dissipation potentials are zero. After the strain/stress condition reaches the yield surface, the ratio jumps to a non-zero value, which depends on ω. In the uncoupled models (fixed value of ω), the ratio of energy dissipation potentials then remains constant throughout the test. The value of this constant can be calculated from Eq.(8) and Eq.(10), as follows:

$$\delta\Phi_p / \delta\Phi_B = \tan(\omega). \tag{19}$$

The ratio may range from 0 to $+\infty$ for ω varying from 0º to 90º. However, according to the analysis presented in Section 4.3, the ratio of dissipation potentials should not be constant during the comminution process: it should increase under higher stresses. The oedometric compression test shows that this ratio, which is expressed by R in [Russell,2011], has a value up to 15.4 when at high breakage. Another experiment also indicates that the breakage dissipation is stress-dependent and that its influence becomes less significant at high stress [Ovalle, Dano and Hicher,2013]. Since the mean effective stress p can be expressed as a function of the breakage parameter B, one can say that the breakage dissipation becomes less important at high breakage.

The internal relationship between the coupling angle ω and breakage B is not obvious, and the assumption we made in Eq.(18) is empirical. Nevertheless, the evolution of the ratio of dissipation potentials that we obtain for a varying ω can to some extent explain the experimental results reported in the literature. The maximum ratio at the strain of 0.5 is around 8.0 in Fig.3, which is less that the results of 15.4 by Russell and thus may indicate that a more sophisticated relationship is needed. Further research will focus on this later point.

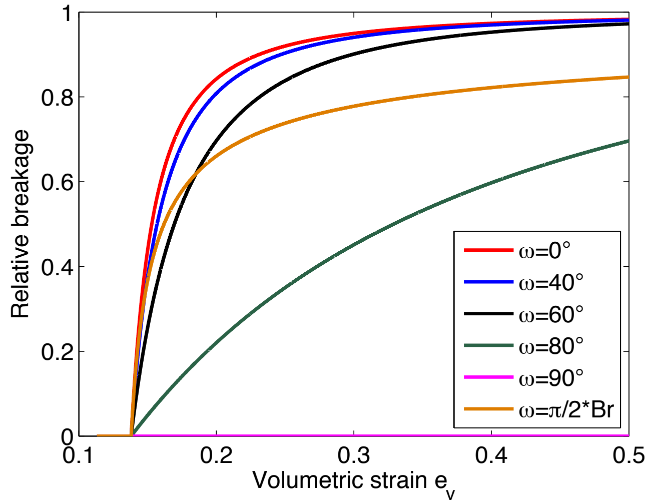

Fig. 2. The effect of the coupling angle ω on the strain-breakage relationship.

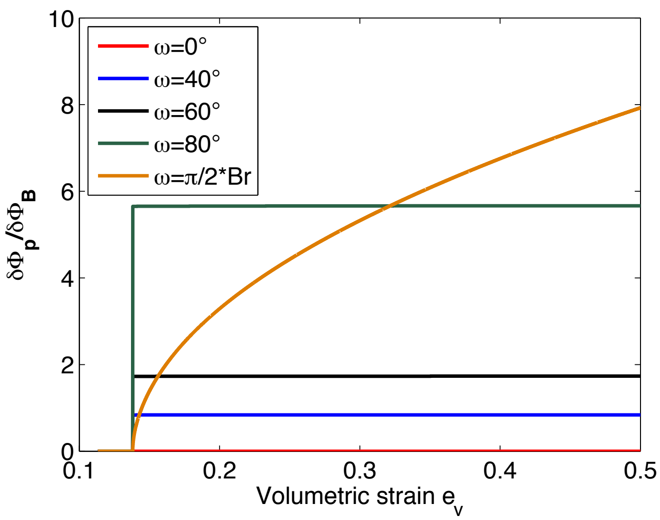

Fig. 3. The effect of the coupling angle ω on $\delta\Phi_p / \delta\Phi_B$.

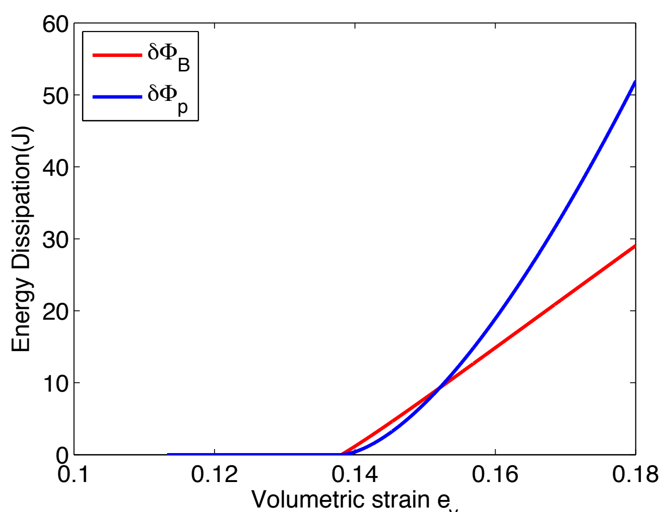

Fig. 4. The relationship between increments of energy dissipation and the volumetric strain

In Fig.4 we see that in our proposed model, breakage dominates energy dissipation when $e_v \leq 0.152$, and then plasticity dominates, which indicates a transition from brittleness to ductility. Fig.5 shows that the breakage is not affected by the coupling angle ω. This is reasonable since from Eq.(11) we know that p and B do not depend on ω.

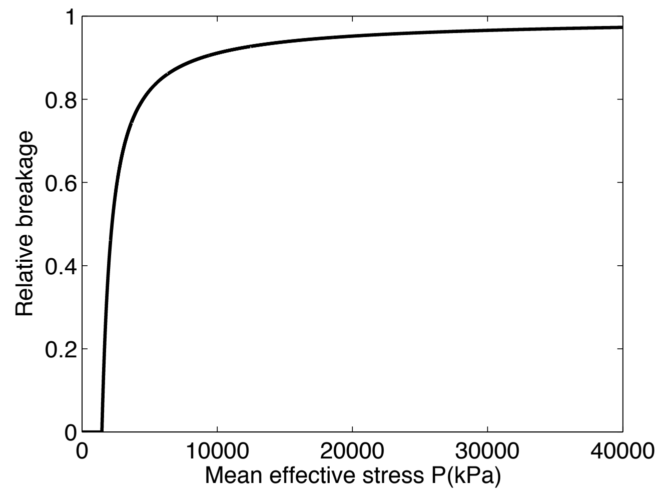

Fig. 5. The effect of the coupling angle ω on the stress-breakage relationship

5. CONCLUSION

In this paper, we propose a model based on the theory of breakage mechanics, in which a friction plasticity parameter is coupled to the breakage parameter. Physically, the relationship between plasticity and breakage translates: (1) the increase of the dissipation induced by breakage in front of that induced by plastic deformation when fragments produced by breakage have rougher surfaces with higher friction angles than the non broken particles; and reversely; (2) the increase of the dissipation induced by plastic deformation in front of that induced by breakage when the multiplication of fragments results in higher particle coordination numbers, shielding effects and higher particle strength. Our modeling hypothesis is supported by experimental observations reported in the literature, and simulations shows that our coupled breakage-plasticity model better captures the brittle-ductile transition observed in granular materials subjected to increasing confining stresses (or volumetric strains). In particular, the model predicts that breakage dissipation dominates at low stress and that plastic dissipation dominates at high stress. Results also confirm experimental observations according to which plastic work is stress-dependent and becomes more significant at high stress. Future work will be dedicated to the proper calibration of the model and to the improvement of the empirical relationship postulated to relate frictional plasticity to particle breakage. The proposed modeling framework is expected improve the simulation of the confined comminution of granular materials, which has many applications in civil engineering, powder technology and the mineral industry.

ACKNOWLEDGEMENTS

Funding to support this research was provided by the U.S. Association of Railroads for the project entitled 'Modeling ballast particle crushing as a phase change'.

REFERENCES

1. Mcdowell, GR, Bolton, MD, Robertson, D. 1996. The fractal crushing of granular materials. *J Mech Phys Solids.* 44(12):2079-2101.
2. Walsh, SDC, Tordesillas, A. 2004. A thermomechanical approach to the development of micropolar constitutive models of granular media. *Acta Mech.* 167(3-4):145-169.
3. Roscoe, KH, Schofield, AN, Thurairajah, A. 1963. Yielding of Clays in States Wetter than Critical. *Geotechnique.* 13(3):211-240.
4. Russell, AR. 2011. A compression line for soils with evolving particle and pore size distributions due to particle crushing. *Geotech Lett.* 1:5-9.
5. Ovalle, C, Dano, C, Hicher, PY. 2013. Experimental Data Highlighting the Role of Surface Fracture Energy in Quasi-Static Confined Comminution. *International Journal of Fracture.* 182(1):123-130.
6. Wang, P, Bakhtiary, E, Ecker, S, Arson, C, Christopher, T, Francis, K. 2015. Discrete Element modeling and analysis of shielding effects during the crushing of a grain. In: *49th US Rock Mechanics/Geomechanics Symposium, 2015*.
7. Tsoungui, O, Vallet, D, Charmet, JC. 1999. Numerical model of crushing of grains inside two-dimensional granular materials. *Powder Technol.* 105(1-3):190-198.
8. Coop, MR, Sorensen, KK, Freitas, TB, Georgoutsos, G. 2004. Particle breakage during shearing of a carbonate sand. *Geotechnique.* 54(3):157-163.
9. Einav, I. 2007. Breakage mechanics - Part I: Theory. *J Mech Phys Solids.* 55(6):1274-1297.
10. Das, A, Nguyen, GD, Einav, I. 2011. Compaction bands due to grain crushing in porous rocks: A theoretical approach based on breakage mechanics. *J Geophys Res-Sol Ea.* 116.
11. Einav, I. 2007. Breakage mechanics - Part II: Modelling granular materials. *J Mech Phys Solids.* 55(6):1298-1320.
12. Wang, P, Arson, C. 2016. Discrete Element Modeling of shielding and size effects during single particle crushing. *Computers and Geotechnics.*(under review).